7.1 Naïve Gaussian Elimination
8.1 The LU Factorization

- Motivating Ax=b: Newton's method for systems of nonlinear equations (pp. 96-99)
- C&K 7.1: Naive Gaussian Elimination
  - See answered problems (1, 2, 3ab, 4, 5, 6, 7abc)

- C&K 8.1: Matrix Factorizations (see pp. 293-302 on LU factorization)
  - See answered problems (1-8)

$$\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$$

Motivation: Newton's Method

(for systems of nonlinear equations, pp.96-99)

In the general case, a system of N nonlinear equations in N unknowns x_i can be displayed in the form

$$\begin{cases} f_1(x_1, x_2, \ldots, x_N) &= 0 \\ f_2(x_1, x_2, \ldots, x_N) &= 0 \\ & \vdots \\ f_N(x_1, x_2, \ldots, x_N) &= 0 \end{cases}$$

Using vector notation, we can write this system in a more elegant form:

$$\mathbf{F}(\mathbf{X}) = \mathbf{0}$$

by defining column vectors as

$$\mathbf{F} = [f_1, f_2, \ldots, f_N]^T$$
$$\mathbf{X} = [x_1, x_2, \ldots, x_N]^T$$

Motivation: Newton's Method

(for systems of nonlinear equations, pp.96-99)

In general, Newton's method uses this iteration:

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} - \left[\mathbf{F}'\left(\mathbf{X}^{(k)}\right)\right]^{-1}\mathbf{F}\left(\mathbf{X}^{(k)}\right)$$

In practice, the computational form of Newton's method does not involve inverting the Jacobian matrix but rather solves the **Jacobian linear systems**

$$\left[\mathbf{F}'\left(\mathbf{X}^{(k)}\right)\right]\mathbf{H}^{(k)} = -\mathbf{F}\left(\mathbf{X}^{(k)}\right) \tag{6}$$

The next iteration of Newton's method is then

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} + \mathbf{H}^{(k)} \tag{7}$$

This is **Newton's method for nonlinear systems**. The linear system (6) can be solved by procedures *Gauss* and *Solve* as discussed in Chapter 7. Small systems of order 2 can be solved easily. (See Problem 3.2.39.)

Motivation: Newton's Method

(for systems of nonlinear equations, pp.96-99)

Example 2 (p. 99)

$$\begin{cases} x + y + z = 3 \\ x^2 + y^2 + z^2 = 5 \\ e^x + xy - xz = 1 \end{cases}$$

$\mathbf{X} = \left[0.1, \quad 1.2, \quad 2.5\right]^T$

for $k = 1$ **to** 10 **do**

$$\mathbf{F} = \begin{bmatrix} x_1 + x_2 + x_3 - 3 \\ x_1^2 + x_2^2 + x_3^2 - 5 \\ e^{x_1} + x_1x_2 - x_1x_3 - 1 \end{bmatrix}$$

$$\mathbf{J} = \begin{bmatrix} 1 & 1 & 1 \\ 2x_1 & 2x_2 & 2x_3 \\ e^{x_1} + x_2 - x_3 & x_1 & -x_1 \end{bmatrix}$$

solve $\mathbf{JH} = \mathbf{F}$

$\mathbf{X} = \mathbf{X} - \mathbf{H}$

end for

Chapter 7.1 (p. 245)

A simple electrical network contains a number of resistances and a single source of electromotive force (a battery) as shown in Figure 7.1. Using Kirchhoff's laws and Ohm's law, we can write a system of linear equations that govern this circuit. If x_1, x_2, x_3, and x_4 are the loop currents as shown, then the equations are

$$\left\{\begin{array}{rcrcrcrcl} 15x_1 & - & 2x_2 & - & 6x_3 & & & = & 300 \\ -2x_1 & + & 12x_2 & - & 4x_3 & - & x_4 & = & 0 \\ -6x_1 & - & 4x_2 & + & 19x_3 & - & 9x_4 & = & 0 \\ & - & x_2 & - & 9x_3 & + & 21x_4 & = & 0 \end{array}\right.$$

Systems of equations like this, even those that contain hundreds of unknowns, can be solved by using the methods developed in this chapter. The solution to the preceding system is

$$x_1 = 26.5 \qquad x_2 = 9.35 \qquad x_3 = 13.3 \qquad x_4 = 6.13$$

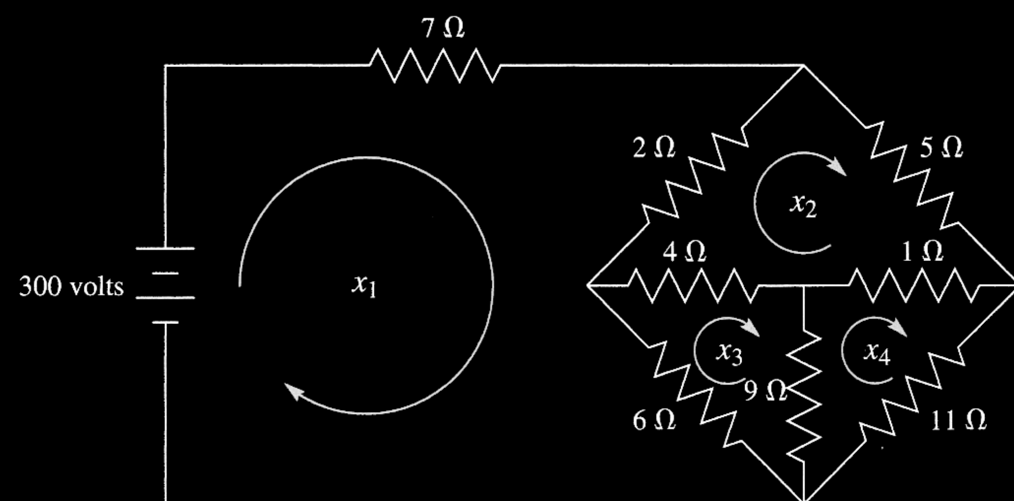

FIGURE 7.1 Electrical network

$$A\,x = b$$

$$\boldsymbol{A\,x = b}$$

$$
\begin{cases}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \\
a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n = b_3 \\
\quad \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\qquad\qquad\quad \vdots \qquad \vdots \\
a_{i1}x_1 + a_{i2}x_2 + a_{i3}x_3 + \cdots + a_{in}x_n = b_i \\
\quad \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\qquad\qquad\quad \vdots \qquad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n
\end{cases}
$$

$$\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$$

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \qquad (1 \leqq i \leqq n)$$

Naïve Gaussian Elimination

$$\begin{aligned}
6x_1 - 2x_2 + 2x_3 + 4x_4 &= 16 \\
12x_1 - 8x_2 + 6x_3 + 10x_4 &= 26 \\
3x_1 - 13x_2 + 9x_3 + 3x_4 &= -19 \\
-6x_1 + 4x_2 + x_3 - 18x_4 &= -34
\end{aligned}$$

Naïve Gaussian Elimination

$$
\begin{aligned}
6x_1 - 2x_2 + 2x_3 + 4x_4 &= 16 \\
- 4x_2 + 2x_3 + 2x_4 &= -6 \\
- 12x_2 + 8x_3 + x_4 &= -27 \\
2x_2 + 3x_3 - 14x_4 &= -18
\end{aligned}
$$

Naïve Gaussian Elimination

$$\begin{aligned}
6x_1 - 2x_2 + 2x_3 + 4x_4 &= 16 \\
- 4x_2 + 2x_3 + 2x_4 &= -6 \\
2x_3 - 5x_4 &= -9 \\
4x_3 - 13x_4 &= -21
\end{aligned}$$

Naïve Gaussian Elimination

$$
\begin{aligned}
6x_1 - 2x_2 + 2x_3 + 4x_4 &= 16 \\
- 4x_2 + 2x_3 + 2x_4 &= -6 \\
2x_3 - 5x_4 &= -9 \\
- 3x_4 &= -3
\end{aligned}
$$

This system is said to be in **upper triangular** form.

Back Substitution

This completes the first phase (**forward elimination**) in the Gaussian algorithm. The second phase (**back substitution**) will solve System (5) for the unknowns *starting at the bottom*. Thus, from the fourth equation, we obtain the last unknown

$$x_4 = \frac{-3}{-3} = 1$$

Putting $x_4 = 1$ in the third equation gives us

$$2x_3 - 5 = -9$$

and we find the next to last unknown

$$x_3 = \frac{-4}{2} = -2$$

and so on. The solution is

$$x_1 = 3 \qquad x_2 = 1 \qquad x_3 = -2 \qquad x_4 = 1$$

Naïve Gaussian Elimination

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\
a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\
\vdots & \vdots & \vdots & & \vdots \\
a_{i1} & a_{i2} & a_{i3} & \cdots & a_{in} \\
\vdots & \vdots & \vdots & & \vdots \\
a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn}
\end{bmatrix}
\begin{bmatrix}
x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_i \\ \vdots \\ x_n
\end{bmatrix}
=
\begin{bmatrix}
b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_i \\ \vdots \\ b_n
\end{bmatrix}
$$

Naïve Gaussian Elimination

After the first step,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ 0 & a_{23} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & a_{i2} & a_{i3} & \cdots & a_{in} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_i \\ \vdots \\ b_n \end{bmatrix}$$

Naïve Gaussian Elimination

first equation as the first **pivot equation** and to a_{11} as the first **pivot element**. For each of the remaining equations ($2 \leqq i \leqq n$), we compute

$$\begin{cases} a_{ij} \leftarrow a_{ij} - \left(\dfrac{a_{i1}}{a_{11}}\right) a_{1j} & (1 \leqq j \leqq n) \\ b_i \leftarrow b_i - \left(\dfrac{a_{i1}}{a_{11}}\right) b_1 \end{cases}$$

The symbol $\leftarrow$ indicates a *replacement*. Thus, the content of the memory location allocated to a_{ij} is replaced by $a_{ij} - (a_{i1}/a_{11})a_{1j}$, and so on. This is accomplished by the following line of pseudocode:

$$a_{ij} \leftarrow a_{ij} - (a_{i1}/a_{11})a_{1j}$$

Note that the quantities (a_{i1}/a_{11}) are the **multipliers**. The new coefficient of x_1 in the ith equation will be 0 because $a_{i1} - (a_{i1}/a_{11})a_{11} = 0$.

Continuing to second equation…

With the second equation as the pivot equation, we compute for each remaining equation $(3 \leqq i \leqq n)$

$$\begin{cases} a_{ij} \leftarrow a_{ij} - \left(\dfrac{a_{i2}}{a_{22}}\right) a_{2j} & (2 \leqq j \leqq n) \\ b_i \leftarrow b_i - \left(\dfrac{a_{i2}}{a_{22}}\right) b_2 \end{cases}$$

k^{th} step of forward elimination

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & \cdots & & \cdots & & \cdots & a_{1n} \\
0 & a_{22} & a_{23} & \cdots & & \cdots & & \cdots & a_{2n} \\
0 & 0 & a_{33} & \cdots & & \cdots & & \cdots & a_{3n} \\
\vdots & \vdots & \vdots & \ddots & & & & & \vdots \\
0 & 0 & 0 & \cdots & a_{kk} & \cdots & a_{kj} & \cdots & a_{kn} \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & a_{ik} & \cdots & a_{ij} & \cdots & a_{in} \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & a_{nk} & \cdots & a_{nj} & \cdots & a_{nn}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_k \\ \vdots \\ x_i \\ \vdots \\ x_n \end{bmatrix}
=
\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_k \\ \vdots \\ b_i \\ \vdots \\ b_n \end{bmatrix}
$$

Naïve GE: Pseudocode

integer i, j, k; **real array** $(a_{ij})_{1:n \times 1:n}, (b_i)_{1:n}$
for $k = 1$ **to** $n - 1$ **do**
  for $i = k + 1$ **to** n **do**
    for $j = k$ **to** n **do**
      $a_{ij} \leftarrow a_{ij} - (a_{ik}/a_{kk})a_{kj}$
    end for
    $b_i \leftarrow b_i - (a_{ik}/a_{kk})b_k$
  end for
end for

Storing Multipliers (instead of zeros)

$$a_{ik} \leftarrow a_{ik} - (a_{ik}/a_{kk})a_{kk}$$

Since we expect this to be 0, no purpose is served in computing it. The location where the 0 is being created is a good place to store the multiplier. If these remarks are put into practice, the pseudocode will look like this:

integer i, j, k;   **real** $xmult$;   **real array** $(a_{ij})_{1:n\times 1:n}$, $(b_i)_{1:n}$
for $k = 1$ **to** $n - 1$ **do**
    for $i = k + 1$ **to** n **do**
        $xmult \leftarrow a_{ik}/a_{kk}$
        $a_{ik} \leftarrow xmult$
        for $j = k + 1$ **to** n **do**
            $a_{ij} \leftarrow a_{ij} - (xmult)a_{kj}$
        end for
        $b_i \leftarrow b_i - (xmult)b_k$
    end for
end for

Back Substitution

At the beginning of the back substitution phase, the linear system is of the form

$$\left\{\begin{array}{rcl}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots & \cdots + & a_{1n}x_n = b_1 \\
a_{22}x_2 + a_{23}x_3 + \cdots & \cdots + & a_{2n}x_n = b_2 \\
a_{33}x_3 + \cdots & + & a_{3n}x_n = b_3 \\
\ddots & \vdots & \vdots \\
a_{ii}x_i + a_{i,i+1}x_{i+1} + & \cdots + & a_{in}x_n = b_i \\
\ddots & \vdots & \vdots \\
a_{n-1,n-1}x_{n-1} & + & a_{n-1,n}x_n = b_{n-1} \\
& & a_{nn}x_n = b_n
\end{array}\right.$$

Back Substitution

The back substitution starts by solving the nth equation for x_n:

$$x_n = \frac{b_n}{a_{nn}}$$

Then, using the $(n-1)$th equation, we solve for x_{n-1}:

$$x_{n-1} = \frac{1}{a_{n-1,n-1}} \left(b_{n-1} - a_{n-1,n} x_n \right)$$

Back Substitution

We continue working upward, recovering each x_i by the formula

$$x_i = \frac{1}{a_{ii}}\left(b_i - \sum_{j=i+1}^{n} a_{ij}x_j\right) \qquad (i = n-1, n-2, \ldots, 1)$$

Here is pseudocode to do this:

integer i, j, n; **real** *sum*; **real array** $(a_{ij})_{1:n\times 1:n}, (x_i)_{1:n}$
$x_n \leftarrow b_n/a_{nn}$
for $i = n-1$ **to** 1 **step** -1 **do**
    $sum \leftarrow b_i$
    for $j = i+1$ **to** n **do**
        $sum \leftarrow sum - a_{ij}x_j$
    end for
    $x_i \leftarrow sum/a_{ii}$
end for

Summary

(1) The basic **forward elimination** procedure using equation k to operate on equations $k+1, k+2, \ldots, n$ is

$$\begin{cases} a_{ij} \leftarrow a_{ij} - (a_{ik}/a_{kk})a_{kj} & (k \leqq j \leqq n,\ k < i \leqq n) \\ b_i \leftarrow b_i - (a_{ik}/a_{kk})b_k \end{cases}$$

Here we assume $a_{kk} \neq 0$. The basic **back substitution** procedure is

$$x_i = \frac{1}{a_{ii}}\left(b_i - \sum_{j=i+1}^{n} a_{ij}x_j\right) \qquad (i = n-1, n-2, \ldots, 1)$$

(2) When solving the linear system $\boldsymbol{Ax} = \boldsymbol{b}$, if the true or exact solution is $\boldsymbol{x}$ and the approximate or computed solution is $\widetilde{\boldsymbol{x}}$, then important quantities are

error vectors	$\boldsymbol{e} = \widetilde{\boldsymbol{x}} - \boldsymbol{x}$
residual vectors	$\boldsymbol{r} = \boldsymbol{A}\widetilde{\boldsymbol{x}} - \boldsymbol{b}$

LU Factorization Example (supplements chalkboard)

Numerical Example

The system of Equations (2) of Section 7.1 can be written succinctly in matrix form:

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 16 \\ 26 \\ -19 \\ -34 \end{bmatrix}$$

Furthermore, the operations that led from this system to Equation (5) of Section 7.1, that is, the system

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 16 \\ -6 \\ -9 \\ -3 \end{bmatrix}$$

Matrix Interpretation

$$MAx = Mb \tag{4}$$

where M is a matrix chosen so that MA is the coefficient matrix for System (3). Hence, we have

$$MA = \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix} \equiv U$$

which is an upper triangular matrix.

Column 1

The first step of naive Gaussian elimination results in Equation (3) of Section 7.1 or the system

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & -12 & 8 & 1 \\ 0 & 2 & 3 & -14 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 16 \\ -6 \\ -27 \\ -18 \end{bmatrix}$$

This step can be accomplished by multiplying (1) by a lower triangular matrix $\boldsymbol{M}_1$:

$$\boldsymbol{M}_1 \boldsymbol{A} \boldsymbol{x} = \boldsymbol{M}_1 \boldsymbol{b}$$

where

$$\boldsymbol{M}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

Column 2

To continue, step 2 resulted in Equation (4) of Section 7.1 or the system

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 4 & -13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 16 \\ -6 \\ -9 \\ -21 \end{bmatrix}$$

which is equivalent to

$$\boldsymbol{M}_2 \boldsymbol{M}_1 \boldsymbol{A} \boldsymbol{x} = \boldsymbol{M}_2 \boldsymbol{M}_1 \boldsymbol{b}$$

where

$$\boldsymbol{M}_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & \frac{1}{2} & 0 & 1 \end{bmatrix}$$

Again, $\boldsymbol{M}_2$ differs from an identity matrix by the presence of the negatives of the multipliers in the second column from the diagonal down.

Column 3

$$\boldsymbol{M}_3\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{A}\boldsymbol{x} = \boldsymbol{M}_3\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{b}$$

where

$$\boldsymbol{M}_3 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -2 & 1 \end{bmatrix}$$

Now the forward elimination phase is complete, and with

$$\boldsymbol{M} = \boldsymbol{M}_3\boldsymbol{M}_2\boldsymbol{M}_1$$

we have the upper triangular coefficient System (3).

Recognizing "L"

$$\begin{aligned} A &= M^{-1}U \\ &= M_1^{-1}M_2^{-1}M_3^{-1}U \\ &= LU \end{aligned}$$

Since each M_k has such a special form, its inverse is obtained by simply changing the sig
of the negative multiplier entries! Hence, we have

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ \frac{1}{2} & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 3 & 1 & 0 \\ 0 & -\frac{1}{2} & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ \frac{1}{2} & 3 & 1 & 0 \\ -1 & -\frac{1}{2} & 2 & 1 \end{bmatrix}$$

It is somewhat amazing that L is a unit lower triangular matrix composed of the multiplier
Notice that in forming L, we did not determine M first and then compute $M^{-1} = L$. (Wh

Verifying $LU=A$

It is easy to verify that

$$\boldsymbol{LU} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ \frac{1}{2} & 3 & 1 & 0 \\ -1 & -\frac{1}{2} & 2 & 1 \end{bmatrix} \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix}$$

$$= \begin{bmatrix} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{bmatrix} = \boldsymbol{A}$$

We see that $\boldsymbol{A}$ is **factored** or **decomposed** into a unit lower triangular matrix $\boldsymbol{L}$ and a upper triangular matrix $\boldsymbol{U}$.